# DRUG-SCREENING SOFTWARE GOES COMMERCIAL

*Can You Imagine . . .*

. . . an algorithm that promises to transform new drug research by rapidly suggesting candidate molecules.

MOLDYN'S COMMERCIAL PLANS FOR ITS COMPUTER ALGORITHM INCLUDE PARTERNERING WITH LEADING PHARMACEUTICAL COMPANIES AND A COMPUTATIONAL CHEMISTRY SOFTWARE FIRM.

Advances in the pharmaceutical industry can be painfully slow and costly. Typically, it takes an average of 15 years and nearly $500 million to bring just one new drug from the laboratory bench to the pharmacy shelf.[1]

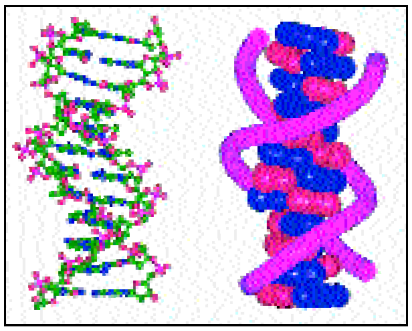
In an effort to expedite drug development, researchers have turned to computational chemistry, a branch of theoretical science that uses digital computers to model systems of chemical interest. But even this computerized technique is time consuming. For example, a full all-atom simulation of just two interlocking molecules can consume hundreds of hours of computer time, even on supercomputers.

Moldyn, Inc. (Arlington, VA), developed a computer algorithm that reduces the time needed to model the dynamics of large molecular systems. The company's algorithm, MBO(N)D[2], promises to transform new drug research, helping find new cures faster. Moldyn, a subsidiary of Photon Research Associates, Inc. (San Diego, CA), developed this technology using BMDO-funded modeling methods designed to simulate the dynamics of large space-based structures.

Because it increases computational speed, MBO(N)D will make the discovery of new drugs and the development of new materials through computational techniques more practical. Tests of the algorithm show that it simulates the dynamics of large molecules (10,000 atoms) up to 50 times faster than conventional all-atom modeling techniques. With further refinements, the algorithm could even be applied to even larger molecules (10,000 to 100,000 atoms) at speeds 100 to 1,000 times faster than all-atom approaches.

Moldyn received an Advanced Technology Program award from the National Institute of Standards and Technology to help bring this technology to the pharmaceutical industry. In this project, the company and its partners will refine the algorithm for commercial use. Moldyn's partners in the project include leading pharmaceutical companies, a computational chemistry software firm, and leading academics in the field of computational chemistry.

The company plans to market the MBO(N)D algorithm as a stand-alone software package and as an interface module link to software already on the market. The stand-alone package targets developers of new drugs and materials, while the interface module targets software firms.



■ Moldyn's algorithm can simulate DNA (pictured above right) 50 times faster than all-atom modeling techniques (pictured above left).

## ABOUT THE TECHNOLOGY

MBO(N)D accelerates computational speed without affecting chemical and physical realism through a technique known as substructuring, which combines atoms into interacting groups of rigid and flexible bodies. The algorithm also filters out small-scale motions that do not affect the overall behavior of the molecule. These two innovations reduce the number of system variables and allow the simulation to be computed over a smaller number of time steps.

[1]Pharmaceutical Research and Manufacturers Association. 1996. The drug development and approval process. World Wide Web at http://www. phrma.org/charts/approval.html.

[2]MBO(N)D stands for multibody order(n) dynamics. Multibody refers to the method of combining the molecules in a series of substructures; order(n) refers to the number of variables in the model. In conventional simulations, the number of variables equals the number of objects squared ($n^2$). MBO(N)D reduces the number of variables to the number of objects (n).